



chain nodes :

6 7 8 9 22

ring nodes :

1 2 3 4 5 10 11 12 13 14 15 16 17 18 19 20 21

chain bonds :

2-8 3-6 5-9 6-7 9-22 13-22 15-16

ring bonds :

1-2 1-5 2-3 3-4 4-5 10-11 10-15 11-12 12-13 13-14 14-15 16-17 16-21 17-18 18-19
19-20 20-21

exact/norm bonds :

1-2 1-5 2-3 2-8 3-4 4-5 5-9 6-7 9-22 13-22

exact bonds :

3-6 15-16

normalized bonds :

10-11 10-15 11-12 12-13 13-14 14-15 16-17 16-21 17-18 18-19 19-20 20-21

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:CLASS